Multithreaded Implicitly Dealiased Pseudospectral Convolutions

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Pseudospectral simulations

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- The nonlinearity becomes a convolution:

$$(F * G)_k = \sum_{k_1,k_2} F_{k_1} G_{k_2}\, \delta_{k,k_1,k_2}.$$

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- For non-centered data, $*(F, G, H) = F * (G * H)$.

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- For centered data, $*(F, G, H) \neq F * (G * H)$.

FFT-based convolutions

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- Non-centered data is padded from length N to length $2N$.
- Centered data is padded from length $2N-1$ to length $3N$.

Implicit Zero-padding

Implicit padding involves using a separate work array to compute the DFT:

$$f_x = \sum_{k=0}^{2N-1} \zeta_{2N}^{xk} F_k, \quad F_k = 0 \text{ if } k \geq N$$

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$$f_{2x} = \sum_{k=0}^{N-1} \zeta_N^{xk} F_k$$

and

$$f_{2x+1} = \sum_{k=0}^{N-1} \zeta_N^{xk} (\zeta_{2N}^{x} F_k)$$

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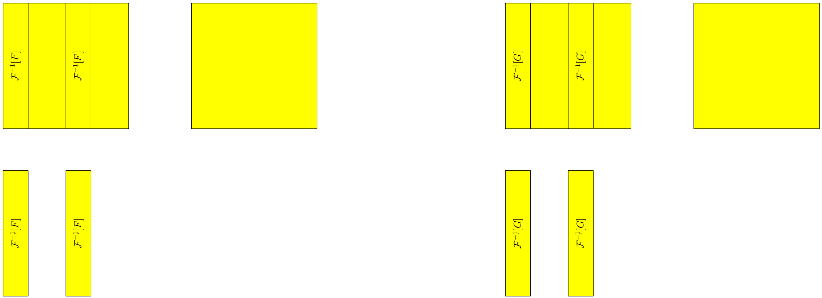

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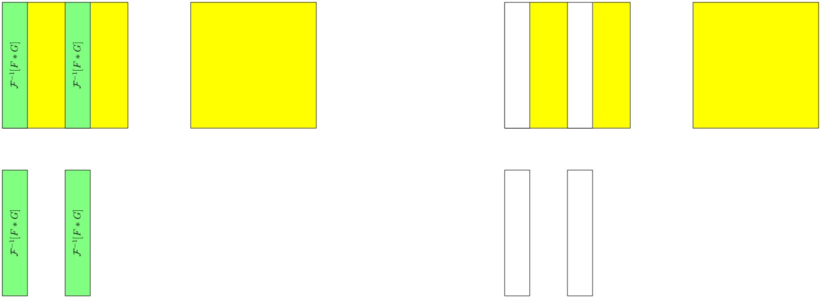

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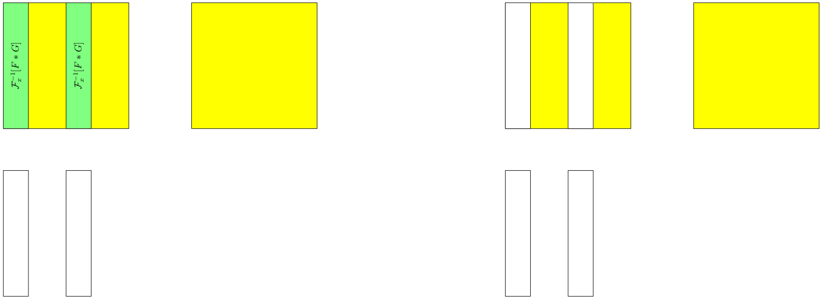

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Memory requirements

Work memory required for an n-dimensional non-centered convolution:

n	Explicit	Implicit
1	$2N_x$	$2N_x$
2	$6N_xN_y$	$2N_xN_y + 2PN_y$
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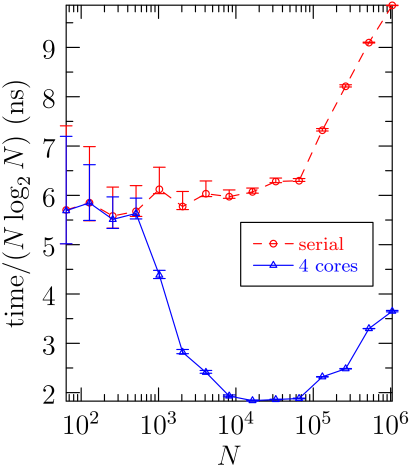
Work memory required for an n-dimensional centered convolution:

n	Explicit	Implicit
1	$2N_x$	$2N_x$
2	$5N_xN_y$	$2N_xN_y + PN_y$
3	$19N_xN_yN_z$	$4N_xN_yN_z + 2PN_xN_y$

Performance: multiple threads



Non-centered 1D convolution.

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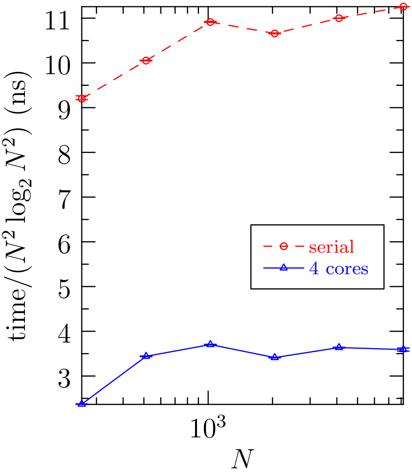

Non-centered 2D convolution.

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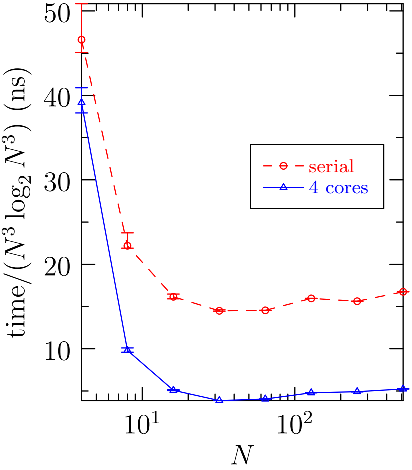
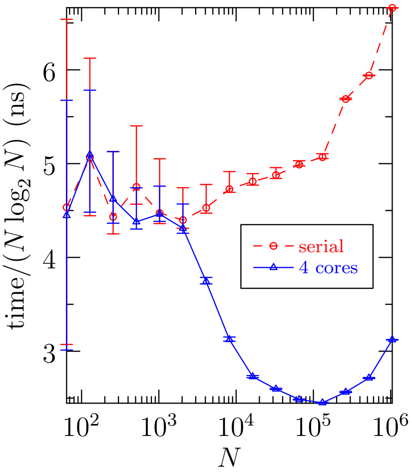


Non-centered 3D convolution.

Performance: multiple threads



Centered 1D convolution.

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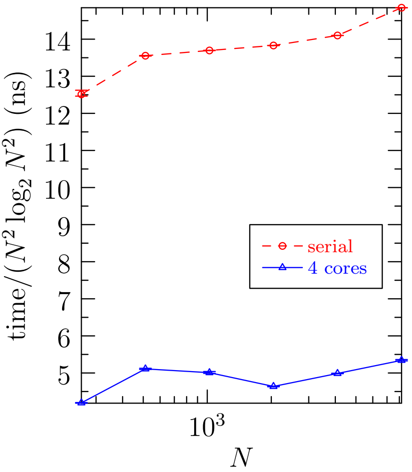

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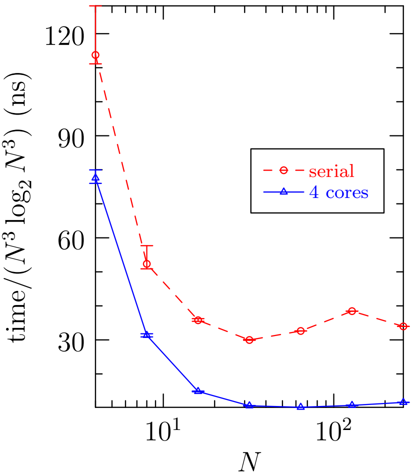

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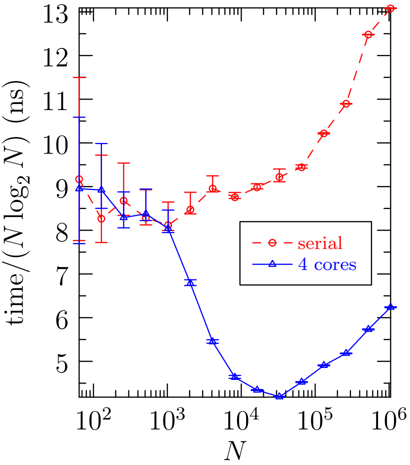
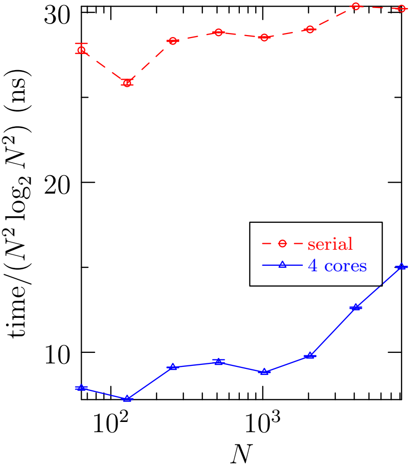


Centered ternary 1D convolution.

Performance: multiple threads



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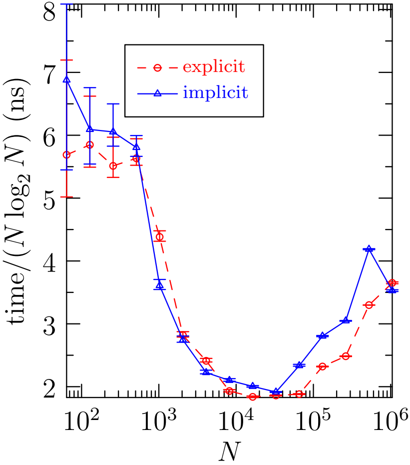
- Three-dimensional convolutions on four cores are about 3.5 times as fast.

Performance: explicit vs. implicit



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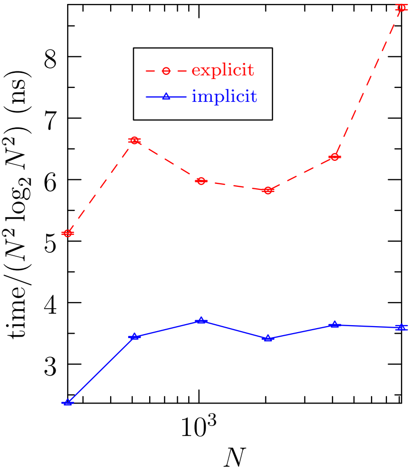

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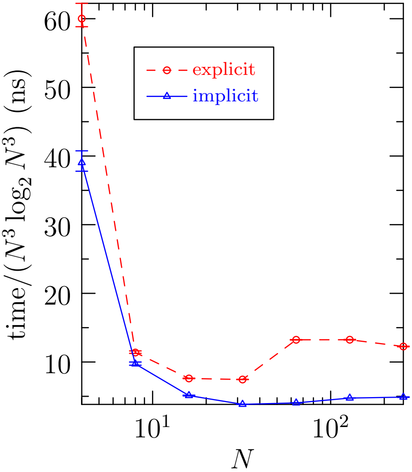

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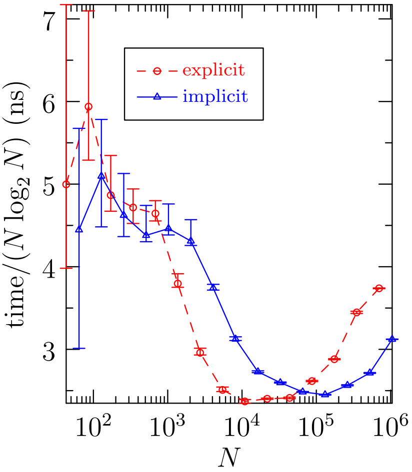

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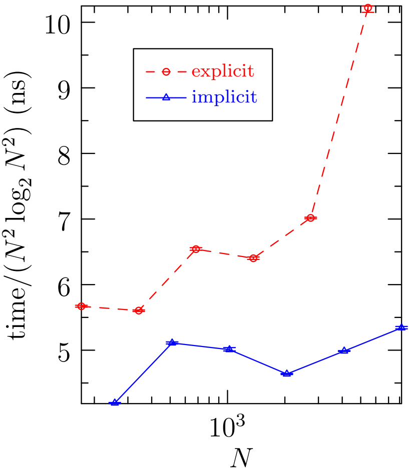

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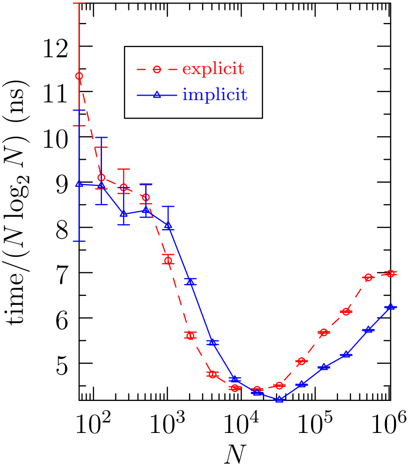

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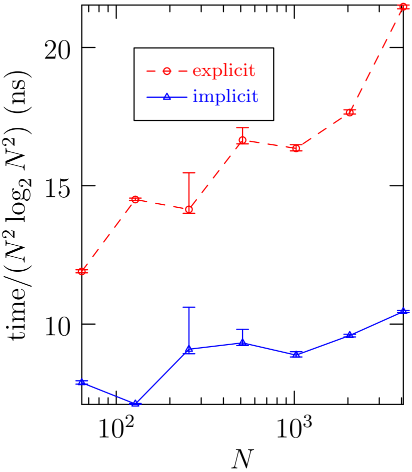

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- The implicit method had a speedup of up to 3.6 on four cores, while the explicit method sped-up of up to a factor of 3.
- The implicit method is around twice as fast as the explicit method for multidimensional convolutions.

Usage example

Computing the nonlinear source of the 2D incompressible Navier–Stokes equations in a vorticity formulation, which appears in Fourier space as

$$\sum_{\mathbf{p}} \frac{p_x k_y - p_y k_x}{|\mathbf{k}-\mathbf{p}|^2}\omega_{\mathbf{p}}\omega_{\mathbf{k}-\mathbf{p}},$$

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One also has the option of passing work arrays to `conv2`, `which can then be used elsewhere.`

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- The algorithm has been successfully implemented on a shared-memory architecture with only a small increase in work memory.
- Convolution algorithms are available for complex non-centered data and centered Hermitian-symmetric data in 1D, 2D, and 3D.
- Ternary convolution algorithms are available for centered Hermitian-symmetric in 1D and 2D.

Future work

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- Add additional routines, such as convolutions on real data, self-convolution, correlations, etc.

Resources

FFTW++:
http://fftwpp.sourceforge.net

Asymptote:
http://asymptote.sourceforge.net

Malcolm Roberts:
http://www.math.ualberta.ca/~mroberts